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Effect of pressure on the magnetic and structural properties of Fe_5SiB_2 compound

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Abstract:

Magnetic and structural parameters of tetragonal Fe_5SiB_2 compound was studied in applied magnetic field up to 7 T and hydrostatic pressure up to 6 GPa in temperature ranging from 2 K up to T_C = 844 K. The temperature dependence of saturated magnetization was measured and described by analytical equation. The decrease of saturated magnetization of dlnM/dp = -1.5 10^{-2} GPa^{-1} was observed. The bulk modulus of 124 GPa was determined by means of high pressure X-ray diffraction. Low temperature spin-reorientation transition was observed and small negative dependence of the transition temperature with respect to pressure was established.

Key words: A. intermetallics; A. functional alloys; B. magnetic properties;B. mechanical properties; hydrostatic pressure; bulk modulus;

Introduction:

In recent years the search for new materials suitable for preparation of rare-earth free permanent magnet has led to renewed interest in the magnetic properties of Fe compounds with anisotropic crystal structure which can promise sizeable magnetic anisotropy. The Fe_5SiB_2 phase was discovered in 1960 by B. Aronsson and I. Engström. The compound crystalizes in the tetragonal crystal structure of Cr_5B_3 type with lattice parameters a = 5.43 Å and c = 10.33 Å. The Fe atoms occupy two different crystallographic positions - 16l and 4c [1]. Newer literature presents slightly different lattice parameters 5.55 Å and 10.34 Å [2, 3, 4, 5], although in all this cases the samples were crushed and annealed as pressed pellets after initial preparation by arc melting. The easy axis magnetic anisotropy with magnetic moment along the c axis was observed at room temperature by Möessbauer experiment [1]. The spin reorientation transition was observed at a temperature of 170 K [1, 3] and the magnetic ground state is characterized by easy plane anisotropy. The effects of substitution of Fe and Si atoms by Co, Mn and P or S were studied [2] in hope of improving the application potential of the compound as a permanent magnet. The spin reorientation transition is highly sensitive to the chemical substitution. The transition temperature decreases with substitution and the compound shows easy axis anisotropy down to the lowest temperature. The experimentally observed behaviour was confirmed and further extended by theoretical calculation [4]. The fixed spin moment calculation and volume variation presented in [4] showed that the absolute value of magneto-anisotropy energy (MAE) is decreasing with increasing unit cell compression as well as with

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decreasing magnetic moment and suggested important differences between the roles of lattice parameters change and electron count in case of chemical substitutions. Change of sign of MAE was predicted around 20 GPa. These results motivated us to study the magnetic and structural properties of Fe_5SiB_2 by means of applying external hydrostatic pressure, which allowed us to further asses the effect of pure volume change on the magnetic properties. In addition to pressure effect the temperature dependence of both crystal lattice parameters and magnetization are reported.

Experimental:

Studied samples were prepared by arc-melting of constituent elements in protective Ar atmosphere. The melted ingot was turned upside-down several times to ensure homogeneity. The resulting sample was checked by EDX and XRD to confirm the Fe_5SiB_2 crystal structure. The volume of additional impurity discovered on XRD pattern was below 3%. The impurity diffraction peaks correspond to the Fe_3Si structure.

The magnetic properties were measured under hydrostatic pressure up to 1 GPa in a piston-cylinder miniature CuBe pressure cell [6] optimised for MPMS instrument (Quantum Design). Daphne mineral oil was used as a pressure transmitting medium. The pressure was determined at low temperature with a Pb sensor and the temperature correction was used to calculate pressure at the respective temperatures discussed in this paper.

The lattice parameters were studied under quasi hydrostatic pressure up to 6 GPa at room temperature. The table top XRD instrument with Ag micro focused radiation with installed Paris-Edinburgh pressure cell was used [7]. NaCl powder was mixed with the powdered sample and inserted in the pressure cell. The pressure was determined from the known pressure dependence of NaCl lattice parameters. The XRD pattern were analysed by least square fitting of the calculated diffraction pattern and the pressure dependence of the lattice parameters of Fe_5SiB_2 were determined.

The temperature dependence of the lattice parameters at ambient pressure was measured from room temperature down to 10 K on a powdered sample using Cu $K\alpha_{1,2}$ radiation. The obtained diffraction patterns were analysed by Rietveld refinement with the help of FullProf software [8].

Results and discussion:

The prepared samples were studied by XRD in order to determine the structure parameters and to determine the purity of the samples. The as-cast sample showed a small amount of the impurity phase (less than 3%). The lattice parameters of the main phase were determined to be a = 5.5196 Å and c = 10.247 Å at room temperature using a least square fit of the observed Bragg peak positions. The space group is I4/mcm where the Fe atoms occupies two crystallographic positions 4c and 16l and Si and B lie on 4a and 8h position, respectively. The X-ray diffraction results are in agreement with previously published structural data [2].

The magnetic properties were characterised by measurement of magnetization isotherms in applied magnetic field up to 7 T at several temperatures. The resulting temperature dependence of $M_s(T)$ was plotted in fig. 1 and fitted by empirical expression derived by Kuz'min [9]:

$$M_s = M_0 \left[1 - s \left(\frac{T}{T_C} \right)^{\frac{3}{2}} - (1 - s) \left(\frac{T}{T_C} \right)^{p} \right]^{\beta} \quad (1)$$

where M_0 is the spontaneous magnetization at 0 K, $\beta = 0.365$ was taken as a critical exponent corresponding to the 3D Heisenberg model and s and p are free parameters of the model.

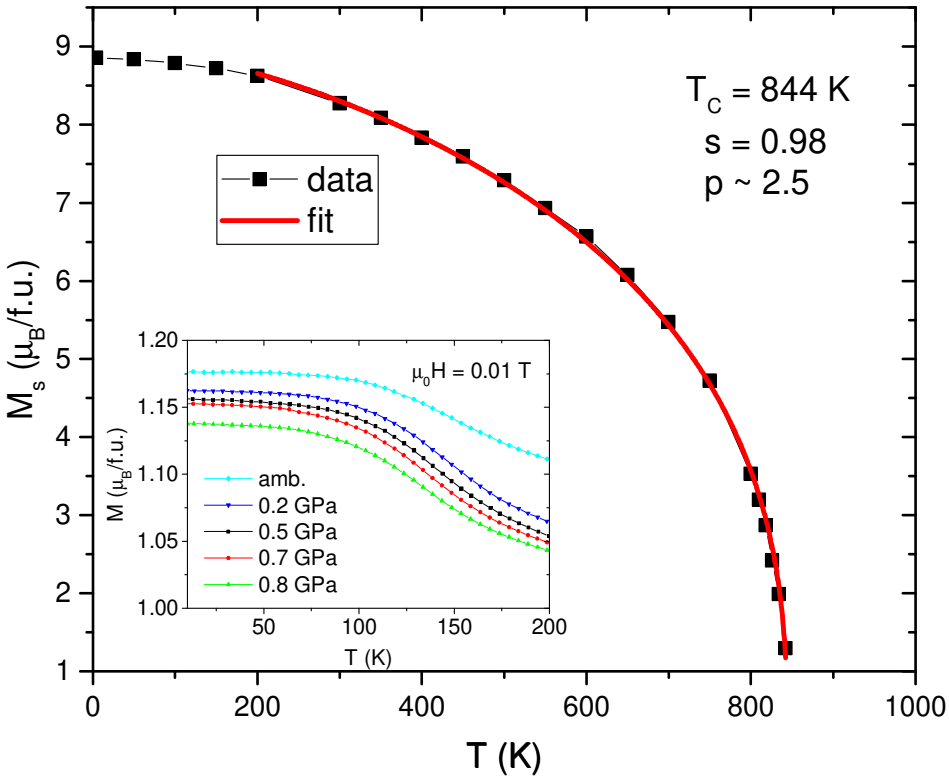

Fig. 1. – Temperature dependence of spontaneous magnetisation determined from M vs. H measurement at different temperatures in magnetic field up to 7 T. The line is a fit to the data according the empirical expression developed by Kuz'min [9].

The Curie temperature was determined to be 844 K and the saturated magnetisation M_0 was fitted to 9.0 μ_B/f.u.. The best fit was obtained for temperatures above 150 K, which suggests that below the spin-reorientation transition a different set of parameters is necessary. Indeed, a spin reorientation transition has been reported to occur around 170 K in earlier studies [1, 3]. It is also worth to note, that although the p parameter converged to a value of 2.5 the s parameter is close to 1 which makes the second term in (1) negligible.

The magnetization with respect to temperature was measured in low magnetic field of 0.01 T as well, which allowed us to observe the spin-reorientation transition manifested as an increase of magnetization at 140 K (temperature determined as an extreme of first derivative of magnetization with respect to temperature). We did not observe the peak like anomaly reported previously [3]. This difference is caused by the isotropic orientation of grains in the measured polycrystalline samples and possibly different degree of structural ordering due to various method of sample preparation.

The structural parameters were further studied upon applying external hydrostatic pressure at room temperature.

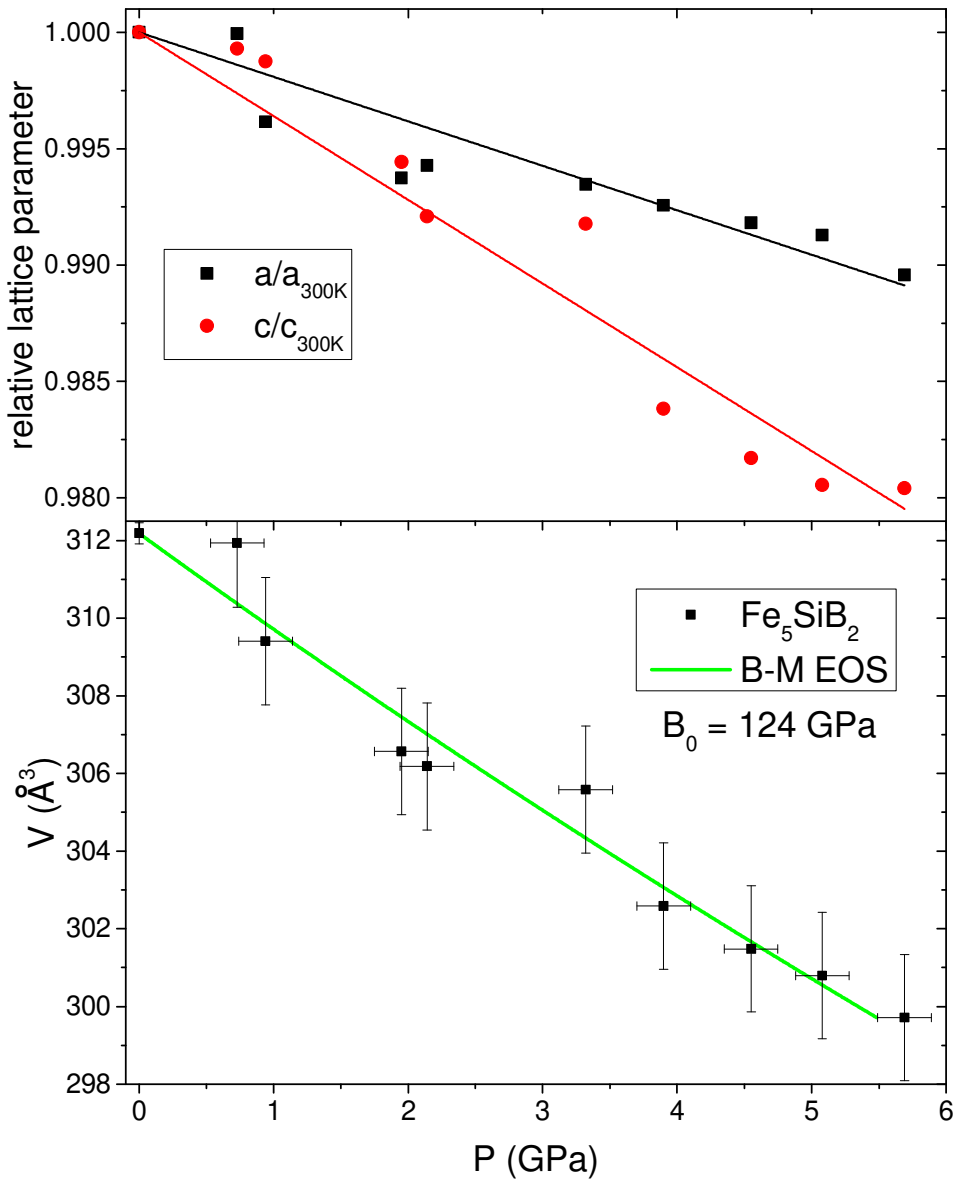

Fig. 2. –The relative lattice parameter a/a_{300K} and c/c_{300K} (a_{300K} = 5.5196 Å and c_{300K} = 10.247 Å) and the V-P diagram determined using XRD under pressure at room temperature. The obtained data was fitted by Birch-Murnaghen equation of state (green line).

The pressure dependence of the lattice parameters was determined and a linear decrease of both a (0.2%/GPa) and c (0.4%/GPa) was observed. The obtained values of volume with respect to pressure (see fig. 2.) were fitted by second order Birch-Murnaghan equation of state. The best fit was obtained for a bulk modulus of 124±4 GPa which is smaller than the values for Fe_5Si_3 or pure Fe but is comparable to values reported for other Fe binary alloys [10, 11]. It is worth to note a comparison with the thermal expansion of the lattice. The lattice parameters obtained by XRD measurements at several temperatures, below 300 K, are presented in fig. 3. The lattice parameter a shows a very small linear decrease from the room temperature value of 5.5196 Å down to 140 K and at lower temperatures the value levels off at about 99.8 % of the room temperature value. The lattice parameter c is constant within the experimental error in the whole studied temperature region.

Present results of thermal expansion agree well with data published in literature [2, 3] and demonstrate the anisotropic character of the unit cell variation versus temperature. Fig. 3 presents the temperature evolution of the unit cell volume from 10 to 300K a reduction of 0.3 % is observed upon cooling the sample corresponding to a mean thermal expansion of 1 10^{-5} K^{-1}.

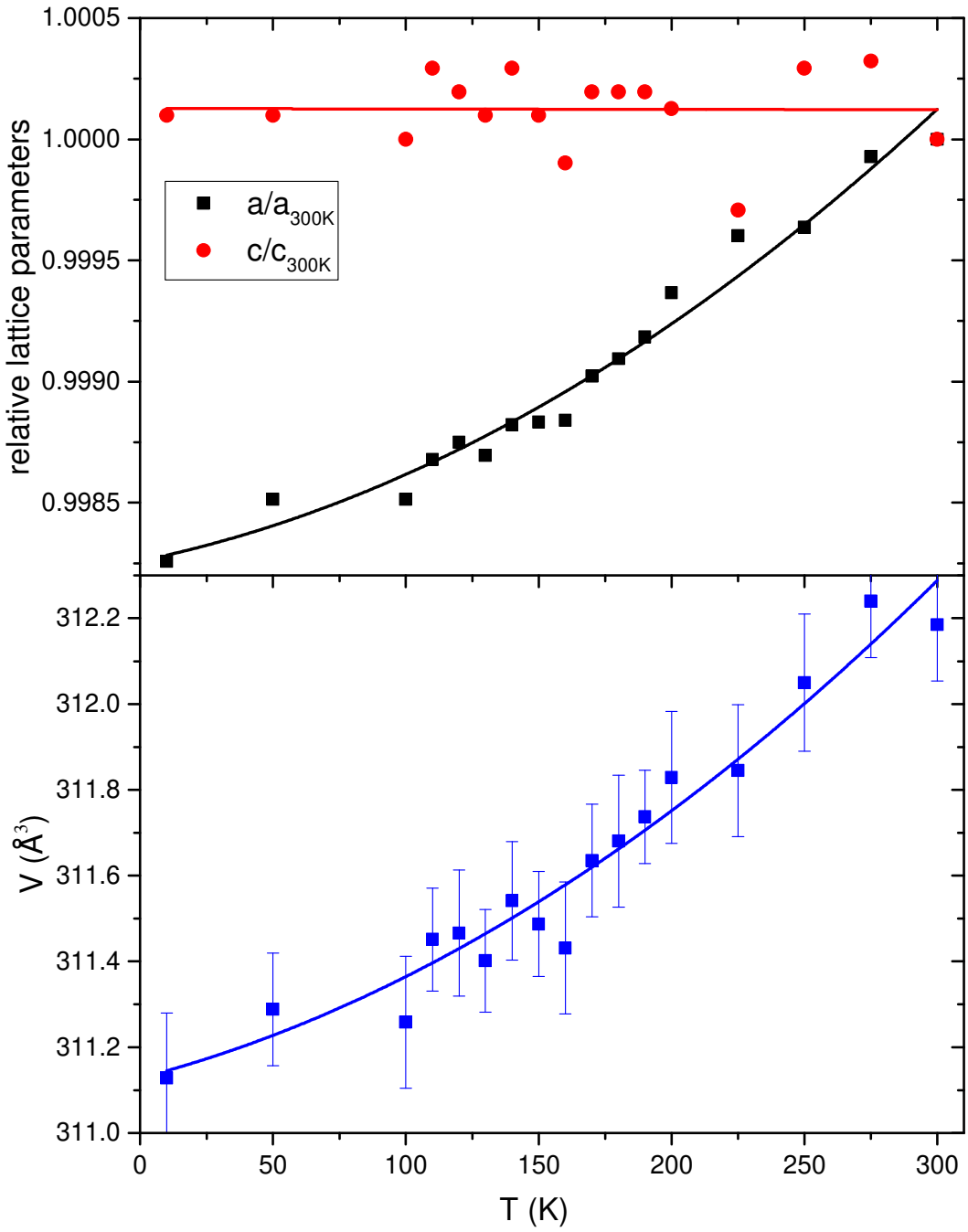

Fig. 3. – Temperature dependence of relative lattice parameter a/a_{300K} and c/c_{300K} (a_{300K} = 5.5196 Å and c_{300K} = 10.247 Å) and unit cell volume.

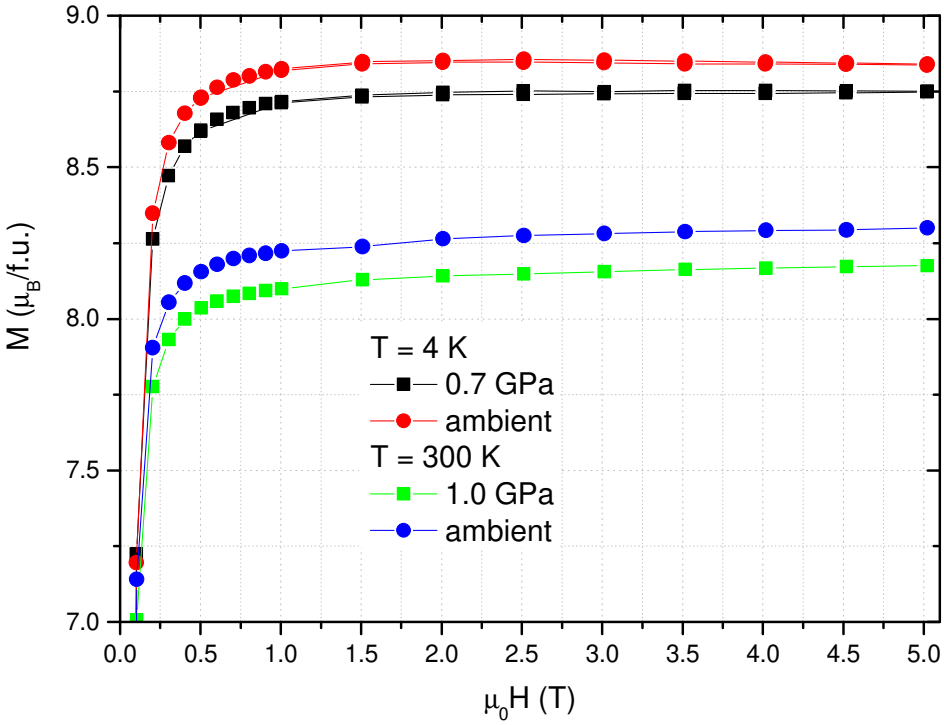

Fig. 4. – Magnetization isotherms measured in applied pressure and ambient pressure at 4 K and 300 K

The magnetic properties were studied in applied pressure up to 1 GPa in order to experimentally correlate the evolution of lattice and magnetism. The magnetization isotherms were measured at several temperatures in applied hydrostatic pressure (see fig. 4). The saturated magnetization shows significant decrease with increasing pressure. The dlnM/dp = -1.5 10^{-2} GPa^{-1} at 4 K as well as at 300 K. The observed value of dlnM/dp is higher than the value observed for pure Fe -4.5 10^{-3} GPa^{-1}, but smaller than values observed for iron binary alloys like Y_2Fe_{17} and others [12, 13, 14]. From the above discussed X-ray diffraction study, we estimate the volume changes corresponding to the applied pressure. The determined bulk modulus can be used to determine the volume dependence of the magnetization as $-B_0 dlnM/dP = V_0 dlnM/dV = 1.9$ at 300 K.

Despite the fact that the measurement was performed on a bulk polycrystalline piece, we were able to detect the spin-reorientation transition with a change from easy *c*-axis to easy plane anisotropy as a broad anomaly on the magnetization versus temperature curve in low applied magnetic field (see the inset of Fig. 1). The effect of pressure was visible as a small decrease of the transition temperature form 139 K at ambient pressure to 134 K at applied pressure of 0.8 GPa which corresponds to a volume change of 0.67 % of V_0. Such behaviour shows that the pressure promotes the easy axis anisotropy although much higher pressure would be needed to suppress the transition completely. The results are in general agreement with theoretical prediction presented by M. Werwinski et al. [4] however some differences can be observed due to the choice of larger equilibrium volume V_0 used for the theoretical calculation.

Conclusions:

We have studied the magnetic and structural properties of Fe_5SiB_2 under applied hydrostatic pressure as well as their temperature dependence. The lattice parameters decrease under applied pressure with the c axis being more sensitive than the a axis, which led to different dependence of c/a parameter with respect to pressure or temperature. The determined bulk modulus is 124 GPa. The magnetic properties were studied from the point of view of the pressure dependence of both the spin reorientation transition and magnetization. The saturated magnetization in the polycrystalline sample was reached above a magnetic field of 1 T at 4 K. The application of pressure led to a decrease of the maximum magnetization and small susceptibility can be observed in magnetic field above 1 T. The same effect of pressure on the magnetization was observed at 300 K as well, which is in agreement with the relatively high Curie temperature of 844 K. The presented results show a relatively small effect of pressure on the magnetic properties as compared to substitution. The $-B_0 dlnM/dP$ is equal to 1.9 as determined from our measurement. We can obtain the value of 17.2 for magnetization and volume of Fe_4CoSiB_2 at 300K and slightly smaller value of 5.5 are obtained in case of P substitution in place of Si for Fe_5PB_2 studied in [2] which is much higher than $-B_0 dlnM/dP$ determined from the measurements presented in this article. The influence of the unit cell volume and/or the c/a ratio on the magnetic properties do not show strong magneto-structural interaction and emphasize the importance of electron count in the case of chemical doping. Pressures around 20 GPa would be needed to supress the spin reorientation transition if the linear pressure dependence of transition temperature is supposed.

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